
APPENDIX A

BREAKOUT SESSION RESULTS

I. MATERIALS AND MANUFACTURING – SESSION A

GROUP SUMMARY

Issues

In order to achieve the SECA goals, the following technology issues received the largest number of votes:

- Metallic interconnects
- Optimize fabrication technology
- New stack designs
- Better materials for seals that are low cost and easy to fabricate into the stack
- Reducing stack operating temperatures to below 700°C to allow use of bare metallic interconnects

R&D Opportunities

The R&D opportunities were categorized into three header topics. The following are the header topics and the corresponding R&D opportunities that received a multiple number of votes:

Advanced Integrated Fabrication Technology

- Single-step SOFC fabrication technique
- Develop low-cost thin-film fabrication/ manufacturing techniques

Component Development

- Low temperature development $\leq 800^{\circ}\text{C}$
- Development and investigation of metal interconnect technology

New Stack Design

- New cheap stack design to minimize interconnects and seals
- New stack designs

Actions

The group's blend of industry, academia, government and national laboratory personnel produced several in-depth technical discussions from a theoretical point of view as well as a "real world perspective." These proved to be a very valuable exchange and dialogue for all the participants. Given the timing constraints, it was only possible to develop specific actions for the top three opportunities.

Low Temperature Component Development:

- Mechanistic studies of electrode kinetics
- Optimize performance of mixed conducting cathodes
- Develop a direct oxidizing anode

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- Oxidation resistant anode
 - Modify anode to control ΔT due to internal reforming
 - Investigation of commercially available alloys for metallic interconnects
 - Cathode side surface treatments on commercially available metallic interconnect materials
 - Investigation of developmental alloys for metallic interconnects

Investigate and Develop Metal Interconnect Technology:

- Interconnect designs that minimize material use
- Investigation of the interconnect and electrode interface
- Explore thermal spray technique
- Control and optimization of sintering of ceramic multi-layers

Advanced Fabrication Technologies:

- Manufacturing cost estimation studies
- Increase mechanical strength of electrode support (or SOFC stack)

In addition to identifying the engineering, development, and research actions, a table was prepared indicating a consensus on the amount of time required to resolve each identified action. In all cases but one, the amount of time required was in the three to six year timeframe. This agrees with the anticipated SECA schedule.

MATERIALS AND MANUFACTURING - SESSION A

PARTICIPANTS

NAME	AFFILIATION
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* = Presenter for report-out

Materials and Manufacturing – Session A: Opportunities Database

<ul style="list-style-type: none"> • Design interconnects alloy that forms a conducting scale • Improved BOP/system integration • Integrate experiments and modeling to minimize sintering and expansion stresses in co-fired ceramic layers • Aqueous processing and fabrication of SOFC materials (where feasible) • Develop metallic interconnect supported design and fabrication process • Identification of new, high performance, lower cost materials. • Develop new multiplayer fabrication capabilities for cofiring • Search/test new materials for seals 	<ul style="list-style-type: none"> • Chromium-free metallic interconnect • Cheap protective coatings for metallic interconnects • Develop viable electrolyte with 10x higher O^{2-} conductivity than YSZ • Develop lower temperature materials • Develop lower cost thin film manufacturing (no UHV) • New anodes/cells that can use hydrocarbon fuels • New, highly electro-active electrodes and development of electrode-supported cells • Development of single-step firing of cells • Single step cell fabrication technology 	<ul style="list-style-type: none"> • Manufacturing cost models • Design for manufacture • Cell stack design • Identify/quantify trade-offs between: pore size dist/amount, gas flow, SOFC performance, and mechanical properties • Develop reliable seals and prove new designs • New electrode materials • Develop cell materials capable of high power density at 700°C and below • Develop new stack designs to simplify manufacturing 	<ul style="list-style-type: none"> • High temperature corrosion of metal interconnects and interfaces • New stack designs • Identify/develop alloys for interconnects • Develop improved extrusion and molding technology for complex parts • Identify and develop durable, high-temperature metal-based interconnects • Custom formulation of metal interconnects • New methods for high temperature, multi-material joining and sealing • Identify and develop seal material/design systems 	<ul style="list-style-type: none"> • Search/test alloys for interconnects • Investigate novel stack designs • Stack modeling • Methods for low cost, high speed deposition of SOFC stack materials • Develop new materials having increased ionic conductivity at reduced temperatures • Develop manufacturing technology which makes stack production cost low
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Materials and Manufacturing – Session A: Issues

(K = Vote for Priority Topic)

<ul style="list-style-type: none"> Given a good fuel cell? How does one verify – technical test issues K Rapid cooldown technique thermal designs Activation potential Sulfur poisoning of anode Complicated thin film/coating technology New stack designs K K K K Innovative stack design 	<ul style="list-style-type: none"> Concurrent operation of metallic plates at operating temperature of ionic conducting ceramics Better materials for seals low cost, easy to fabricate into stack K K K K Durable sealing (stack design/bonding agent) K K K Development of thinner cell components to lower amount of material per cell Hydrogen as fuel, new anode Stack must survive rapid thermal cycling 	<ul style="list-style-type: none"> Interconnect inventory High working temperature 800°C → 700°C Bi-polar supported (metallic) SOFC for cost reduction Cathode performance Expensive cathode materials Synergistic impact of R&D on issues Greater, more available body of knowledge and data (knowledge transfer includes from other fields) Basic knowledge and data relating to interconnects Multiple materials currently require multiple fabrication steps/ processes, single step process needed Low-cost manufacturing of tri-layer cells Too many manufacturing steps K 	<ul style="list-style-type: none"> Metallic interconnects K K K K K K K K Metals do not like to live at temperatures where conducting ionic ceramics like to operate so SOFC operating temperature must drop below ≈700°C to allow use of bare metal K K K K K K Lower temperature materials K K Materials with higher conductivities at lower temperatures Cells/stacks manufacturing process flexibility Need materials/sealing geometries that can survive extreme thermal stresses of transient operation/fast startup Quality consistency in the ability to mass manufacture ceramic cells K K K Quality of materials and fabrication processes Refinement, in process technology for making cells Electrolyte (thin film) deposition and sintering K 	<ul style="list-style-type: none"> Complicated manufacturing procedures requiring multiple firings of ceramics SOFC materials are not computer components Optimize fabrication technology K K K K K K K K K K Small scale (size) extrusion technology needed K Development of multi-material co-firing to lower manufacturing costs Low cost, efficient materials Ability of SOFCs to follow load Single SECA goals (identify intermediate niches) 	<ul style="list-style-type: none"> Lack of anodes capable of high fuel conversion with minimal prereforming (maximized efficiency) Req. use of high cost, dissimilar material properties materials that cause integration challenges Long term chemical compatibility data
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Materials and Manufacturing – Session A: R&D Opportunities

(K = Vote for Priority Topic)

ADVANCED INTEGRATED FABRICATION TECHNOLOGY	COMPONENT DEVELOPMENT	NEW STACK DESIGN
<ul style="list-style-type: none"> Single step SOFC fabrication technique K K K K K K K K Develop low-cost thin-film fabrication / manufacturing techniques K K K Integrated cell/stack design with fabrication process development 	<ul style="list-style-type: none"> Low temperature development <800 K K K K K K K K K K Identify new, novel seals and separators for test and evaluation K Development and investigation of metal interconnect technology K K K K K K K K K K 	<ul style="list-style-type: none"> New stack design(s) K K K New stack, cheap design to minimize inter-connects and seals K K K K K K Conduct trade-off studies, i.e., temperature/materials K Modeling to enable new design development and cost K Design economic simulation model of effect of new designs on manufacturing cost Investigate material vs. design function trade-offs K Miniaturizations K Expand knowledge base of SOFC reliability under arbitrary operating conditions

Materials and Manufacturing – Session A: What Are the Actions Needed to Take Advantage of the Opportunities?

R&D OPPORTUNITY	ACTIONS	TYPE OF ACTION	0-3	3-6	6-10	INDUSTRY	ACADEMIA	NATIONAL LABS
LOW TEMPERATURE COMPONENT DEVELOPMENT	• Mechanistic studies of electrode kinetics	R	X				A	
	• Optimize performance of mixed-conducting cathodes	D	X			I		N
	• Develop direct oxidizing anode	R	X	X			A	
	• Oxidation resistant anode	R	X	X			A	N
	• Modify anode to control ΔT due to internal reforming	D/E	X	X		I		N
	• Investigation of commercially available alloys	D	X				A	
	• Cathode side surface treatment on commercially available alloys	D	X	X		I		N
	• Investigation of developmental alloys	D	X	X		I	A	N
INVESTIGATE AND DEVELOP METAL INTERCONNECT TECHNOLOGY	• Interconnects designs that minimize material use	E	X	X				N
	• Investigation of interconnect, electrode interface	R	X	X			A	N
	• Explore thermal spray techniques	D	X	X				N
	• Control and optimization of sintering of ceramic multi-layers	R/D	X	X		I		N
ADVANCED FABRICATION TECHNOLOGIES	• Manufacturing cost estimation studies	D/E	X	X		I		N
	• Increase mech. strength of electrode support (or SOFC stack)	D/E	X	X	X	I		N

Key: E = Engineering
D = Development
R = Research

Materials and Manufacturing – Session A: Report-Out

TECHNICAL ISSUES	R&D OPPORTUNITIES	KEY OPPORTUNITIES	ACTIONS
<ul style="list-style-type: none"> • Metallic interconnects • Optimize fabrication technology • Lower temperature materials • Durable seals • New stack designs (current stack designs) 	<ul style="list-style-type: none"> • Component development <ul style="list-style-type: none"> ! Low temperature electrode development ! Develop and investigate metal interconnect technology • New stack design <ul style="list-style-type: none"> ! Minimize interconnects and seals ! Trade-offs driving design of stacks • Advanced integration fabrication technologies <ul style="list-style-type: none"> ! Single-step fabrication technique ! Low-cost thin-film techniques 	<ul style="list-style-type: none"> • Low Temperature Component Development 	<ul style="list-style-type: none"> • Mechanistic studies of electrode kinetics • Optimize performance of mixed-conducting cathodes • Develop direct oxidizing anode • Oxidation resistant anode • Modify anode to control ΔT due to internal reforming • Investigation of commercially available alloys • Cathode side surface treatment on commercially available alloys • Investigation of developmental alloys
		<ul style="list-style-type: none"> • Metal Interconnect Technology 	<ul style="list-style-type: none"> • Interconnects designs that minimize material use • Investigation of interconnect, electrode interface • Explore thermal spray techniques • Control and optimization of sintering of ceramic multi-layers
		<ul style="list-style-type: none"> • Advanced Fabrication Technologies 	<ul style="list-style-type: none"> • Manufacturing cost estimation studies • Increase mech. strength of electrode support (or SOFC stack)

II. MATERIALS AND MANUFACTURING – SESSION B

GROUP SUMMARY

Issues

In order to achieve the SECA goals, the following technology issues received the largest number of votes:

- Fabrication of stacks from cells
- Thin-film manufacturing cost
- Interconnects metal or oxide

While the costs of raw materials is not a major concern now, availability of certain materials (e.g., LSM and YSZ) could be problem down the road if the market takes off.

R&D Opportunities

The R&D opportunities were categorized into five header topics. The following are the header topics and the corresponding R&D opportunities that received a multiple number of votes:

Design

- Develop novel, low-cost cell stack design concepts

Interconnects

- Develop new interconnect alloys from fundamental understanding of oxidation kinetics and oxide conductivity

Fabrication/Manufacturing

- Cost-effective fabrication of high-performance cell stacks including tri-layers, thin electrolyte, electrolyte coating, low temperature, and colloidal deposition
- NDE to enhance manufacturability

Materials Properties

- Develop internally reforming stacks (anode or manifold)
- Develop different anode material for different fuels

Interface

- Fundamental investigations into interfaces-microstructures and catalytic properties
- Investigate novel interlayer for adhesion and chemical protection

Actions

Key action steps were developed for the top three opportunities.

Develop cost-effective fabrication techniques for high performance fuel cell stacks:

- Conduct fundamental studies into why defects occur
- Investigate large scale thin film deposition
- Develop in-situ NDE methods for identifying defects
- Adapt existing ceramic technique for specific fuel cell designs
- Develop low cost interconnect and seals

Develop new interconnect alloys from fundamental understanding of oxidation kinetics and oxide conductivity:

- Examine interface and coatings inter-relations and stability
- Examine stability and electric transport at interface
- Conduct surface modification studies

Develop compact, reliable, low cost fuel cell design concepts:

- Immediately study design as function of performance parameters
- Define cost and performance specifications
- Create ability to evaluate thermal and chemical properties with in-situ diagnostic tools
- Determine effects of high power density on long-term performance
- Build in design review to ensure flexibility to respond to change
- Evaluate transport phenomena
- Evaluate feasibility of internal reforming under multi-fuel conditions

MATERIALS AND MANUFACTURING - SESSION B

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* = Presenter for report-out

Materials and Manufacturing – Session B: Scientific and Technology Issues

(K = Vote for Priority Topic)

MANUFACTURABILITY	INTERCONNECT MATERIALS	COST OF RAW MATERIALS	PERFORMANCE	STACK SYSTEM DESIGN AND INTEGRATION
<ul style="list-style-type: none"> For target power density no high volume, low-cost tri-layer fabrication technology exists K K K K K K Need for system integration of stack components and automated manufacturing Lack of alternatives to the costly EVD process for depositing the electrolyte K Basic understanding of how electrode/electrolyte reliability is affected by colloidal deposition parameters K Fabrication of stacks from cells K K K K K K K K K K K K Thin-film manufacturing cost K K K K K K K K Lack of NDE for manufacturing 	<ul style="list-style-type: none"> Lifetime of interconnect materials Interconnect metal or oxide? K K K K K K K K Lack of inexpensive thermally reliable seals Metal interconnects needed above 650°C 	<ul style="list-style-type: none"> Low demand for LSM, YSE materials Availability of high V, low-cost raw material K 	<ul style="list-style-type: none"> O of 60 to 70% will require 0.85 V/C+; close to theoretical present is 0.7 V/C Slow electrode kinetics at low temperature Limited temperature range Catalysis limiting issues below 700°C Lack of NDE techniques to predict remaining life K K Specific power (W/cm²) K Anode composition and structure to permit full <i>in situ</i> reforming K Hydrocarbon tolerances and poisoning K Design of novel interfaces with minimum resistance K 	<ul style="list-style-type: none"> Thermal management Low cost PEN with controlled morphology electrodes K Need for inexpensive thermal insulation Fuel delivery to all cells in stack Serviceability of complex fuel stack Materials compatibility Settling too soon on tech design Gas manifolding on mass customization of core module Need to recycle address disposal/ recycling of materials from stack Thermal cycling of scaled-up reduced temperature planar stacks

Materials and Manufacturing - Session B: R&D Opportunities

(K = Vote for Priority Topic)

DESIGN	INTERCONNECTS	FABRICATION/ MANUFACTURING	MATERIALS PROPERTIES	INTERFACE
<ul style="list-style-type: none"> Improve thermal cycle Develop measures to shorten start-up K Develop novel, low-cost cell stack design concepts K K K K K K K K ! Compact with improved reliability ! Minimize/eliminate sealing issues 	<ul style="list-style-type: none"> Compliant metallic interconnect K Investigate novel thin-film coatings for metallic interconnects – low cost Develop a) low thermal expansion b) high conductivity material that can survive in both reducing and oxidizing environments Develop new interconnect alloys from fundamental understanding of oxidation kinetics and oxide conductivity K K K K K K K K 	<ul style="list-style-type: none"> Cost-effective fabrication of high-performance cell stacks ! Trilayers ! Low-cost thin electrolyte processing technology ! Develop and scale up electrolyte coating process and thin film stack manufacturing ! Low temperature ! Study colloidal deposition parameters impact on reliability – flaw development during coating/debinding/firing K K K K K K K K K K K K Develop a repetitive manufacturing process Flaw development in co-firing (suppression) NDE to enhance manufacturability K K Develop process models for fabrication K 	<ul style="list-style-type: none"> Lower operating temperatures Solve film adhesion problems Develop different anode material for different fuels K K ! Novel composites for anodes Develop internally reforming stacks (anode +/- manifold) K K K K K K K K Study chemical reactions at all interfaces during the fabrication and operation of electrode-supported thin-film stack K Conduct modeling of material reliability and life-time production NDE of lifetime prediction of stack components Examine long-term dimensional stability of flat plate 	<ul style="list-style-type: none"> Transport across heterogeneous interfaces and electrode architecture performance Fundamental investigations into interfaces-microstructure and catalytic properties K K K K Investigate novel interlayer for adhesion, chemical protection K K K K

Materials and Manufacturing - Session B: Actions

R&D OPPORTUNITY	BRIEF DESCRIPTION OF OPPORTUNITY	TYPE OF ACTION	KEY ACTION STEPS	LEAD ROLES	OTHER POINTS
<ul style="list-style-type: none"> Develop cost-effective fabrication techniques for high performance fuel cell stacks 	<ul style="list-style-type: none"> Multi-cell stack extrusion Long term-new ways to make ceramics Lack of volume is main reason costs of manufacturer is high Dramatic cost reductions are needed. Capital costs of equipment are high <i>In situ</i> firing? Core can participate in long term – trilayers and PENs One-step firing Defects are a problem for reliability Start with simple traditional techniques 	<ul style="list-style-type: none"> R First 3 years use today's process Longer term other methods will be needed 	<ul style="list-style-type: none"> Fundamental studies into why defects occur Investigate large scale thin film deposition – review existing work Develop in-situ NDE methods for identifying defects Adapt existing ceramic technique for specific fuel cell designs Develop low cost interconnect and seals 	<ul style="list-style-type: none"> Industry Longer-term concepts – consortia –NL, U 	<ul style="list-style-type: none"> Do not use material at temperatures higher than you make it
<ul style="list-style-type: none"> Develop new interconnect alloys from fundamental understanding of oxidation kinetics and oxide conductivity 	<ul style="list-style-type: none"> Very difficult problem! Chromium-are there other materials? Compounds Oxides, etc. as coatings? Need scale that is good conductor Lowering temperature can help Coatings are possibility but have own problems 	<ul style="list-style-type: none"> Mostly R and some D 	<ul style="list-style-type: none"> Ongoing throughout program Examine interface and coatings inter-relations and stability Examine stability and electric transport at interface Conduct surface modification studies 	<ul style="list-style-type: none"> National labs and universities Consortium with industrial input 	<ul style="list-style-type: none"> Watch over next 3-5 years
<ul style="list-style-type: none"> Develop compact, reliable low cost fuel cell stack design concepts 	<ul style="list-style-type: none"> Design new stacks “core” Making stacks small involves core design issues Thermal and mass flow in compact SOFC Modify existing stacks “Industry Group” Choice of fuel is key 	<ul style="list-style-type: none"> Core D and R Industry E 	<ul style="list-style-type: none"> Study design as function of performance parameters 1st year Define cost and performance specifications Create ability to evaluate thermal and chemical properties in situ diagnostic tools 	<ul style="list-style-type: none"> Industry lead in design 	<ul style="list-style-type: none"> Need to have ability to change and avoid “lacking in” to particular designs Focus as quickly as possible on limited number of designs

Materials and Manufacturing - Session B: Actions *(Continued)*

R&D OPPORTUNITY	BRIEF DESCRIPTION OF OPPORTUNITY	TYPE OF ACTION	KEY ACTION STEPS	LEAD ROLES	OTHER POINTS
<ul style="list-style-type: none"> Develop compact, reliable low-cost fuel cell stack design concepts (<i>con't</i>) 	<ul style="list-style-type: none"> 	<ul style="list-style-type: none"> 	<ul style="list-style-type: none"> Determine effects of high power density on long term performance Build in design review to ensure flexibility to respond to change Evaluate transport phenomena overtransient long term condition Evaluate feasibility of internal reforming under multi-fuel conditions 	<ul style="list-style-type: none"> 	<ul style="list-style-type: none">

Key: E = Engineering
 D = Development
 R = Research

Materials and Manufacturing – Session B: Report Out

DESIGN AND MANUFACTURING	BREAKOUT SESSION OVERVIEW	MATERIALS	CLOSING REMARKS
<ul style="list-style-type: none"> Design is developed by industry <ul style="list-style-type: none"> ! Design affects manufacturability ! Novel ideas should be explored ! Address transient operations/thermal cycling Near-term – refining tapecasting Long-term – “multi-cell extrusion” 	<ul style="list-style-type: none"> Achieving cost goals is dominating factor Major materials issues <ul style="list-style-type: none"> ! More specific than manufacturing issues at this time 	<ul style="list-style-type: none"> Nature of electrolyte and electrode did not emerge as major issue <ul style="list-style-type: none"> ! Low temperatures, different story (e.g., power densities) ! $T(E)$; A/cm^2 Interconnects are a major area to address <ul style="list-style-type: none"> ! Membrane contacts ! Oxidation 	<ul style="list-style-type: none"> Difficult balance – design do not “lock in” too soon but focus as soon as possible <ul style="list-style-type: none"> ! Design reviews Mobile ↔ stationary fuels

III. FUEL PROCESSING – SESSION A

GROUP SUMMARY

Issues

In order to achieve the SECA goals, the following technology issues received the largest number of votes:

- Catalysis - reduction of the size of processing hardware for multi-fuel
- Operation with little or no water
- Gas contaminant removal or purification
- Very rapid transient response
- Reformer stability during transients
- Fully integrated fuel processor
- Ability to internally reform natural gas

Overall, what is needed is a fully integrated fuel processor with multi-fuel capability that is small and is sulfur tolerant. Also, the reformer must have operational stability during transients, start-up, and shut-down conditions. The critical challenge mentioned repeatedly is either sulfur cleanup or sulfur tolerance. Without resolving this issue, many candidate fuels and markets cannot be considered for solid-state fuel cell system applications.

R&D Opportunities

The R&D opportunities were categorized into five header topics. The following are the header topics and the corresponding R&D opportunities that received a multiple number of votes:

System Development and Demonstration

- System level reformer development
- Development of low-cost, accurate sensors
- Multi-path approach to demonstrate electrochemical reformer

Fuel Characterization

- None

Clean-Up Process

- Develop a liquid phase de-sulfurization system
- Sulfur removal – gas phase H₂S, organic sulfides

Catalyst Development

- Reformer catalyst development
- Catalyst characterization – performance, life, cost
- Combinatorial approaches to catalysts

Modeling

- System modeling to identify optimal strategies for integrating stack and reformer designs
- Transient control, dynamic temperature, and reaction rates in reformer catalysts

Actions

System Level Reformer Development:

- Develop commercial, integrated, reliable reformer
- Develop modular packages for a family of sizes and functions or parameters

Fuel Processor Catalyst Development:

- Determine and characterize catalyst durability vs. fuel and operating conditions
- Improve catalyst yield and efficiency
- Characterize catalysts for sulfur tolerance and fuel consumption
- Develop alternate catalysts via combinatorial approach
- Evaluate sulfur removal techniques in liquid and gas phase
- Define level of sulfur cleanup requirements by fuel
- Evaluate and investigate reaction chemistry
- Evaluate and demonstrate small integrated efficiency reformer
- Maintain data in catalyst database/reformer handbook
- Test method and standard procedures to benchmark designs vs. target requirements
- Evaluate close coupled in-stack reforming
- Evaluate POX and ATR conversion selectivity
- Optimize reformer
- Evaluate integrated system in a remote field location
- Demonstrate catalyst endurance characteristics

System Modeling to Integrate Stack and Reformer Designs:

- Evaluate close-coupled in-stack reforming
- Develop user friendly commercially supported modeling package for reaction kinetics through coupled reformer and stack

The group identified research, development, and engineering actions that would need to be completed within the next 0-5 years and within 5-10 years to achieve the SECA vision. Within the next 5 years much catalyst development and system development activities need to begin. Initially, databases on catalysts and reformers need to be compiled and made available based on characterization and trade-off studies and evaluations. From 5-10 years, system optimization and demonstrations should be stressed.

FUEL PROCESSING - SESSION A

PARTICIPANTS

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* = Presenter for report-out

Fuel Processing – Session A

What Are the Science and Technical Issues to Achieving Vision?

(K = Vote for Priority Topic)

CATALYST ISSUES	FUEL ISSUES	GAS CLEAN-UP	OPERATIONAL ISSUES	COST ISSUES	SYSTEM INTEGRATION
<ul style="list-style-type: none"> Catalyst availability for variety of fuels K Lack of more predictive catalyst design tools Catalysis - Reduction of size of processing hardware for multi-fuel K K K K K Catalyst life K Coking problems K K Electrochemical reformers K Sulfur-tolerance and direct electrochemical oxidation K K ! Stable catalyst (sulfur) ! Rapid start-up ! Partial Ox. Reformer Sulfur removal, sulfur tolerance to reformer catalyst K 	<ul style="list-style-type: none"> Operation with little or no water (gasoline, diesel) K K K K K K Small and efficient P.O. reformer for gasoline and diesel 90% conversion K Direct diesel (multi-fuel) SOFC, Eliminate reformer K Partial oxidation of liquid fuels with oxygen K Feedstock flexible K Logistic fuels – compact, fuel-flexible, rapid response 	<ul style="list-style-type: none"> Active sulfur removal gas phase K Desulfurization technology – needs to be high capacity, without need for hydrogen, compatible with metcaptions and thiophenes Gas contaminant removal (or) purification K K K K Pure hydrogen stream Selective gas separation technologies: oxygen, hydrogen, CO, etc. K 	<ul style="list-style-type: none"> Load following fuel source K 20 to 1 turndown sensors Requirement for very rapid transient response rapid transient resp. K K K K Reformer stability during transients (startup-shut down – ramp) K K K K K Control sensor how do we know when the reformer is deteriorating? Freeze protection Cycling 	<ul style="list-style-type: none"> Low-cost high temperature heat exchangers K Materials of construction (high-temperature) Hydrogen embrittlement Catalyst cost O&M 	<ul style="list-style-type: none"> Fully integrated fuel processor T, heat balance K K K K K Size reduction issues – heat management issues Start-up requirements cold-hot K K Achieving 60-70% efficiency goal without bottom cycle and in volume/wt envelope is challenging Ability to internally reform (in stack) ! Natural gas K K K K Control system K

Fuel Processing – Session A
What Are the R&D Opportunities to Overcome the Issues?
(k = Vote for Priority Topic)

SYSTEM DEVELOPMENT AND DEMONSTRATION	FUEL CHARACTERIZATION	CLEAN-UP PROCESSES	CATALYST DEVELOPMENT	MODELING
<ul style="list-style-type: none"> Develop low cost high temperature heat exchangers k DOE work in high “R” insulations k Development of low-cost, accurate sensors kk Modular control system concepts System-level reformer development kkkkkkkk Microchannel reformers for reduced size and integration Multi-path approach to demonstrate electro-chemical reformer kk Develop low-cost, fully integrated fuel processor module k Operational characterization of “state-of-the-art” fuel processors (Team) 	<ul style="list-style-type: none"> Define and characterize fuels Decide what fuel is best – reference fuels 	<ul style="list-style-type: none"> Sulfur removal – gas phase H₂S, organic sulfides kk Long life regenerable sulfur sorbents – demonstrate Nanoporous ceramic membranes for gas purification Develop a liquid phase De-S system kkk Mixed oxide conductors for fuel processing 	<ul style="list-style-type: none"> Catalyst characterization – performance, life, cost kk Develop multi-fuel single catalyst Reformer catalyst development kkkkkkkk ! Steam reforming ! POX reforming k ! ATR k Regenerable catalyst, also with in-situ gas cleanup Low temperature (400-600°C) catalysts for direct oxidation k Combinational approaches to catalysts kk Nanostructural catalysts Catalyst R&D ! “Dry” reforming ! Sulfur tolerant ! Long life ! Low cost ! Size reduction 	<ul style="list-style-type: none"> Develop reaction kinetics modeling ! Different fuels ! Different water ! Coke formation System modeling to identify optimal strategies for integrating stack and reformer designs kkkk Modeling heat flows Chemical reaction modeling for POX k Fundamentals of hydrocarbon reforming (in-situ, . . .) k Transient control dynamic temperature, temperature and reaction rates in reformer catalysts (chemical modeling) kkk System modeling “optimizations” toward mass customization

Fuel Processing – Session A

What Are the Actions to Take Advantage of the R&D Opportunities?

SYSTEM-LEVEL REFORMER DEVELOPMENT	SYSTEM MODELING TO INTEGRATE STACK AND REFORMER DESIGNS	FUEL PROCESSOR CATALYST DEVELOPMENT	LEAD ROLE(S)
<ul style="list-style-type: none"> • Develop a commercial, integrated, reliable reformer • Modularity – packages/family of sizes and functions (parameters) 	<ul style="list-style-type: none"> • Evaluate close coupled in-stack reforming • Develop user friendly modeling package for reaction kinetics through coupled reformer and stack <ul style="list-style-type: none"> ! Commercially supported platform ! Demonstrate and validate 	<ul style="list-style-type: none"> • Determine, characterize catalyst durability vs. fuel and operating conditions Database (0-5 years) • Improve catalyst yield/efficiency life (Research) • Characterize catalysts for: <ul style="list-style-type: none"> ! S tolerance ! Steam/C ratio (min) ! Fuel composition • Develop alternate catalysts (combinatorial approach) <ul style="list-style-type: none"> ! Lower cost ! Non-noble metal ! 0-5 years: membranes? Benefits/tradeoffs ! Sulfur tolerance removal • Evaluate S removal techniques in liquid and gas phase <ul style="list-style-type: none"> ! Disposable ! Regenerable ! Active • Define level of S clean-up requirements (by fuel) • Evaluate; investigate reaction chemistry (Research, Development) <ul style="list-style-type: none"> ! Liquid fuels ! Steam ! Pox ! ATR ! Electro-chem • Evaluate and demonstrate small integrated efficiency reformer (Engineering, Development) (Gaseous) <ul style="list-style-type: none"> ! Gaseous fuels ! Steam ! Pox ! ATR • 0-5 Years – Maintain data of catalyst database/reformer handbook • Test method and standard procedures to benchmark designs vs. target requirements • Evaluate close coupled in-stack reforming • 0-5 years - Evaluate determine P.O.-sooting, ATR conversion selectivity (temp range) diesel and gasoline JPx • Trade-offs of reformer types by application (Engineering) • 5-10 Years – Optimize reformer (Engineering) • 5-10 Years – Evaluate integrated system in remote field location • Evaluate and demonstrate a small, integrated, eff. reformer (Engineering) • 5-10 years - Demonstrate catalysts endurance characteristics 	<ul style="list-style-type: none"> • Ultimately – industry • Core tech – university and national labs

Fuel Processing - Session A: Report-Out

SCIENCE AND TECHNICAL ISSUES	R&D OPPORTUNITIES	ACTIONS
<ul style="list-style-type: none"> • Cost Issues • Integration <ul style="list-style-type: none"> ! Fully integrated fuel processor • Operational <ul style="list-style-type: none"> ! Reformer stability during transients (startup, shutdown, etc.) • Gas Cleanup <ul style="list-style-type: none"> ! Gas contaminant cleanup (include S) • Fuel Issues <ul style="list-style-type: none"> ! Min S/C ratios • Catalyst Issues <ul style="list-style-type: none"> ! Develop for multi-fuel and size ↓ ! S-tolerance 	<ul style="list-style-type: none"> • Modeling <ul style="list-style-type: none"> ! Reaction kinetics ! Systems modeling • Catalyst Development <ul style="list-style-type: none"> ! New catalysts and characterization of current ! S-tolerance • Clean-Up Processes <ul style="list-style-type: none"> ! S-removal!! ! Other contaminants • System Development <ul style="list-style-type: none"> ! Reformer integration with other components • Fuel characterization 	<ul style="list-style-type: none"> • System Level Reformer Development <ul style="list-style-type: none"> ! Split – gaseous – liquid ! Further – steam, Pox, ATR, Electrochemical (liq) • Fuel Processor Catalyst Development • Systems Modeling • System (0-5 years) <ul style="list-style-type: none"> ! Evaluate, investigate reaction chemistry ! Characterize small reformers ! Database on catalysts and reformers ! Standard procedures for test/targets ! Trade-offs by reformer type and application – list all parameters (soot conversion, others) • System (5-10 years) <ul style="list-style-type: none"> ! Optimize ! Demonstrate • Catalyst Development (0–5 years) <ul style="list-style-type: none"> ! Improve catalyst conv. efficiency and life ! Characterize existing catalysts (S, S/C, etc.) ! Develop alternate catalysts (cost↓, S) ! S cleanup, liq phase ! Membranes • Catalyst Development (5-10 years) <ul style="list-style-type: none"> ! Demonstrate! • Systems Modeling <ul style="list-style-type: none"> ! Evaluate coupled reformer/stack ! Develop user friendly commercially supported modeling for reaction kinetics → coupled reformer/stack

IV. FUEL PROCESSING – SESSION B

GROUP SUMMARY

Issues

In order to achieve the SECA goals, the following technology issues received the largest number of votes:

- Availability of low-cost, small-scale reformers to deal with diesel and logistic fuels
- Deactivation of catalyst
- Internal reforming thermal management and poisoning
- Performance with respect to durability, life, and load following.

R&D Opportunities & Actions

The R&D opportunities were categorized into five header topics. However, the group did not vote on specific opportunities, but instead they voted on the header topics. Therefore, the following are the three header topics that received the most votes with only the first three bullet details presented.

Making Diesel Fuel Processor Work

- Make poison resistant partial oxidation reactor
- Demonstrate a two-stage diesel steam reformer
- Develop liquid fuel processors to remove sulfur

Propane/Natural Gas Fuel Processor as Cheap as Possible

- Develop low-cost, high-efficiency gaseous fuel reformer
- Develop a very inexpensive oxidative reforming unit
- Design for low cost manufacturing

Internal Reforming

- Design and build models for internal reforming stack
- Develop graded anode
- Develop oxidative internal reforming process for natural gas and propane

Actions

The group developed actions from the top three categories of R&D opportunities.

Develop a Compact Fuel Processor for Diesel and Logistics Fuels:

- Novel fuel conversion processes, e.g., advanced oxygen sources for partial oxidation and micro-channels to enhance heat transfer

-
- Fuel pre-processing systems to remove troublesome impurities before they are charged to the fuel processor
 - Anode catalysts that are resistant to sulfur and carbon
 - Advanced balance of plant systems

These activities were categorized as spanning research and development.

Make Light Fuels Processors (Natural Gas, Propane, and Gasoline) as Low Cost and Compact as Possible :

- Thermal integration
- Miniaturization of equipment for 5 kW
- Start by simplifying fuel processors designed for PEM
- Multi-fuel R&D
- Integrated fabrication development
- Lowering components costs through DFMA and other means

These activities were categorized as primarily engineering.

Develop Internal (On-Anode) Reforming Technology:

- Steam reforming and POX
- Lab tests of internal reforming systems and use the data acquired to develop electrochemical and thermodynamic models of processes and obtain fundamental knowledge of them
- Multi-fuel tolerant core module
- Graded anode technology
- Advanced fuel-mixing concepts to facilitate heat transfer and management

Internal reforming was described as the “holy grail” of fuel processing, and activities supporting it are staunchly in the research end of the action spectrum.

FUEL PROCESSING - SESSION B

PARTICIPANTS

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Fuel Processing- Session B: Issues

(K = Vote for Priority Topic)

PERFORMANCE	STACK SENSITIVITY (SULFUR & SALT) POISON	LOW CAPACITY OF SYSTEM	INTERNAL REFORMING	FUEL EFFECT ON FUEL PROCESSOR	FUEL PROCESSING BOP
<ul style="list-style-type: none"> Long-term testing durability K Long life of reformer materials at low cost K Start-up time Load following K 	<ul style="list-style-type: none"> Anode Poisoning <ul style="list-style-type: none"> Salt Sulfur 	<ul style="list-style-type: none"> Difficult for Diesel K Availability of low cost small scale reformer K K K K K K Thermal losses in small systems Reliability at small scale 	<ul style="list-style-type: none"> Poisoning K Cracking Thermal management K K Preconditioning of fuel 	<ul style="list-style-type: none"> Deactivation of catalyst K K K <ul style="list-style-type: none"> Thermal Coking Sooting Poisoning 	<ul style="list-style-type: none"> Sulfur absorption/disposal (filter cartridge) using alkali metal Long life desulfurizer K Water sufficiency

Fuel Processing – Session B: Opportunities

(K = Vote for Priority Topic)

MAKING DIESEL FUEL PROCESSOR WORK kkkkkkkkkk	PROPANE/NATURAL GAS FUEL PROCESSOR AS CHEAP AS POSSIBLE kkkkkkkkkk	INTERNAL REFORMING kkkkkkkk	BALANCE OF PLANT kkk	OTHER ITEMS
<ul style="list-style-type: none"> • Make poison resistant partial oxidation reactor <ul style="list-style-type: none"> - ceramic membrane • Demonstrate a two stage (diesel) steam reformer (fluid-bed/Plug Flow) for 100 kWe system and work backwards down • Liquid fuel processors to remove sulfur—disposable filter-1 gallon can processes 20 gallons of fuel • Come up with a dual catalyst that tolerate sulfur anode and coking • Integrated reformer/heat transfer approach <ul style="list-style-type: none"> - Microchannel - Plate reformers • Fuel preprocessor <ul style="list-style-type: none"> - Remove sulfur - Increase fuel quality • Develop inert, stable materials 	<ul style="list-style-type: none"> • Develop low-cost, high efficiency gaseous fuel reformer • Very inexpensive oxidative reforming unit for natural gas and propane • Design for low cost manufacturing • Integrated fabricate development 	<ul style="list-style-type: none"> • Models for internal reforming stack – design – build • Graded anode development • Oxidative internal reforming process for natural gas and propane • Mixing fuel in cell rather than plug flow to improve internal reforming • Develop a multi-fuel tolerant internal reforming core module (cell) 	<ul style="list-style-type: none"> • Sensors • Materials • Manufacturing • Techniques • Reduce parasitic load 	<ul style="list-style-type: none"> • Accelerated durability testing reformer/stack • Long term materials research and tests • System optimization • Ultra-rich internal combustion engine as POX fuel processor shaft power out quick start • Coking-resistant coating for preconditioner

Fuel Processing – Session B: Actions

FUEL PROCESSOR FOR DIESEL AND LOGISTIC FUELS	ULTRA LOW-COST HIGH EFFICIENCY FUEL PROCESSOR FOR NATURAL GAS AND PROPANE	INTERNAL REFORMING (ON-ANODE)
<ul style="list-style-type: none"> • Novel Processes <ul style="list-style-type: none"> - Ceramic Membrane POX - Integrated heat transfer microchannel /plate reformer - Two stage heavy fuel steam reformer - Materials resistant to impurities - Pilot plant - At 20 kW • Fuel Pre-processing <ul style="list-style-type: none"> - Liquid phase desulfurization - Better ways to remove sulfur during processing • Materials research to develop anode catalyst to resist sulfur and carbon • BOP <ul style="list-style-type: none"> - 5 KW - Systems integration - Perform R&D on components with integration in mind - Thermally integrated reforming 	<ul style="list-style-type: none"> • Develop low cost, high efficiency gaseous fuel reforming <ul style="list-style-type: none"> - Steam - POX - Other - Thermally integrated reforming - Build at 5 kW - Starting point. Simplify fuel processors designed for PEM stacks - Multi-fuel R&D - Integrated fabrication development - Design low cost manufacturing 	<ul style="list-style-type: none"> • Most effort is on steam reforming, could look at POX as well • Lab scale experimentation <ul style="list-style-type: none"> - Modeling - Thermal - Chemical - Electro-chemical • Multi-fuel tolerant core module • Graded anode • Fuel mixing

Fuel Processing – Session B: Report-Out

(K = Vote for Priority Topic)

ISSUES	OPPORTUNITIES	ACTIONS	COMMENT
<ul style="list-style-type: none"> • Dealing with diesel and logistic fuels • Lack of demonstrated internal reforming capability • Low capacity • Sensitivity of stack to sulfur, soot and salt • Lack of demonstrated performance durability • Reliability, long life, start up, multiple fuels, • Diesel and logistic fuels makes problem much more difficult • Internal reforming not clear you can be successful • Low capacity • Sulfur, soot, salt • Performance 3 	<ul style="list-style-type: none"> • Developing a compact (5-20 kW) diesel fuel processor K K K K K K K K K K • Light fuels (natural gas, propane, gas) as low cost and compact as possible K K K K K K K K K K • Internal reforming (on-anode) K K K K K K K K • Developing a compact diesel fuel processor full preprocessor, sulfur removal, coking pox, steam • Light fuels processor mass manufacturing to get low cost reliability, POX, steam, novel • Internal 	<ul style="list-style-type: none"> • Diesel and logistic fuel <ul style="list-style-type: none"> - Novel processing - Fuel pre-processing - Anode to resist sulfur and carbon - BOP • Natural gas, propane and gasoline <ul style="list-style-type: none"> - Thermal integration - Small size - DFMA • Internal reforming <ul style="list-style-type: none"> - Lab tests/modeling - Graded anode - Fuel mixing 	<ul style="list-style-type: none"> • Requirement of heavy fuels complicates vision <ul style="list-style-type: none"> - Other goals at risk • Alternate strategy – focus on natural gas for market introduction • Early stage R&D on heavy fuels

V. MODELING AND SIMULATION

GROUP SUMMARY

Modeling and simulation issues for fuel cells are best discussed by considering issues that impact the fundamental cell, component, stack, or system, or crosscut through all of these scales.

Issues

The following issues received the most votes:

- Validation/benchmark data for models/modeling
- Barrier – posing of critical questions answerable by appropriate models
- Electro-chemical reaction rates and mechanisms
- Lack of suitable multi-physics engineering models
- Diversity of scales hinders Computational Fluid Dynamic (CFD) applications in multi dimensions at stack level.
- Total life cycle cost/performance analysis and optimization

R&D Opportunities

The R&D opportunities were categorized into five header topics. The following are the header topics and the corresponding R&D opportunities that received a multiple number of votes:

Crosscutting

- Joint validation benchmarks where more than one group develops, characterizes, tests, and models
- Model SOFC operations: start-up, part-load, shut-down (load following)
- Define precisely what validation data are needed and get it
- Perform uncertainty analysis on fuel cell models at all levels (focus on numerical errors)

Cell/Fundamental

- Development of fundamental multi-dimensional models with emphasis on electrochemical and kinetic transport aspects
- Determine electro-chemical rates and mechanisms: measure and model
- Develop 3D fundamental multi-scale model for micro-structural analysis and design

Component

- None

Stack

- Develop coupled multi-dimensional multi-physics engineering model for stack with benchmark problem set

System

- Build reliability model of SOFC system

Actions

To take advantage of the top three R&D opportunities, the following actions should be carried out:

Develop Models for the Cell and for the Stack:

- Multi-dimensional, multi-physics
- Develop benchmark problem set (for stack)
- Electrochemical, kinetic, transport emphasis for cell

Benchmark Development:

- Developed and characterize benchmark cells
- Test to provide data on benchmark cells
- Models will be developed for benchmark cells

Model SOFC Operation (Start Up, Part Load, Shut Down):

- Industries establish the off-design conditions and requirements
- Develop coupled transient models
- Validate the models

MODELING AND SIMULATION

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Modeling and Simulation: What Are the Science and Technical Issues to Achieving the Vision?

(K = Vote for Priority Topic)

CROSSCUTTING ISSUES	CELL/FUNDAMENTAL MODELS	COMPONENT MODELS	STACK MODELS	SYSTEM MODELS
<ul style="list-style-type: none"> • Validation/benchmark data for models/modeling kkkkkkkkk • Barrier—posing of critical questions answerable by appropriate models kkkk • Cost functions (accurate) {lack thereof} kk • Dynamic communication with materials and manufacturing groups (lack thereof) kk • Lack of education and training on fuel cell technologies k • Connection and communication between modeling (scales of modeling) groups k • Lack of public domain software k • Need real-life values for model parameters k • Lack of operating codes and standards for design modeling • Lack of benchmark for verification 	<ul style="list-style-type: none"> • Electro-chemical reaction rates and mechanisms kkkk • Lack modular cell-level physical-mathematical models for transport processes k • Simulating direct Internal reformation transport phenomena k • There is a need for greater detailed information from models • Need constitutive equations for mirco/fundamental models 	<ul style="list-style-type: none"> • Better models for fuel processing kk 	<ul style="list-style-type: none"> • Lack of suitable multi-physics engineering models <ul style="list-style-type: none"> - Thermal, electro-chemical, transport coupling kkkkkkk • Diversity of scales hinders computational fluid dynamic (CFD) applications in multi-dimensions at stack level kkk • Lack of a public domain research code for multi-dimensional modeling at the stack level k • Methods for determining fabrication stress k • Simulating indirect internal reforming transport phenomena • Interface properties for PEN material and seals • Reliability model • Need for handbook approach for stack 	<ul style="list-style-type: none"> • Total life cycle cost/performance analysis and optimization <ul style="list-style-type: none"> - Model cost/ maintenance trade-offs - Fuel cell fabric. Auxiliary equipment installation kkk • Reliability/ Availability/ Maintainability (RAM) models

Modeling and Simulation: What Are the R&D Opportunities to Overcome the Issues?

(K = Vote for Priority Topic)

	CROSSCUTTING	CELL /FUNDAMENTAL	COMPONENT	STACK	SYSTEM
Validation Opportunities	<ul style="list-style-type: none"> Define precisely what validation data that we need and get it (database) K K K K K 	<ul style="list-style-type: none"> Material databases electrochemical and thermal and failure data Develop tests and test standards for measuring material properties especially interfacial properties 			
Computation Opportunities (Modeling)	<ul style="list-style-type: none"> Model SOFC Operations: Start-up, part-load, shut-down (Load following) K K K K K K Handbook of Fuel Cell Model equations and thermal papers K Thermoeconomic design studies K Develop efficient numerics for such complex problems K Perform uncertainty analysis on fuel cell models at all levels (focus on numerical errors) K K 	<ul style="list-style-type: none"> Development of fundamental multi-dimensional models which emphasizes on: electrochemical, kinetic transport aspects on the cell level. K K K K K K Develop 3D fundamental multi-scale model for microstructural analysis and design K K 	<ul style="list-style-type: none"> Fuel reformation models K 	<ul style="list-style-type: none"> Develop coupled multi-dimensional multi-physics engineering model for stack with benchmark problem set K K K K K K K Coordinated joint effort to develop a multi-dimensional robust, public domain computer code for stack K Develop modeling tools for predicting residual stress due to fabrication 	<ul style="list-style-type: none"> Build reliability model of SOFC system K K Build diagnostic model of SOFC system Fuel cell cost algorithms K
Joint Validation/ Computation Opportunities	<ul style="list-style-type: none"> Benchmarks <ul style="list-style-type: none"> more than one group develop and characterize <u>same</u> cell design more than one group test above and provide detailed data more than four groups model Define metrics or figure of merit and how they relate to one another K 	<ul style="list-style-type: none"> Determine electro-chemical rates and mechanisms: measure and model K K K Model Equation Development <ul style="list-style-type: none"> Research on kinetics (electrochem and reforming) Propose and test models Publish all results 		<ul style="list-style-type: none"> Understand failure mechanisms in stack/cell K 	

Modeling and Simulation: What Are the Actions to Take Advantage of the R&D Opportunities?

R&D OPPORTUNITY	ACTIONS 0-5 YEARS	ACTIONS 5-10 YEARS	LEAD ROLE	OTHER ISSUES
DEVELOP MODELS FOR STACK AND CELL <ul style="list-style-type: none"> Multi-dimensional, multi-physics With benchmark problem set (for stack) Electrochemical, kinetic, transport emphasis for cell 	<ul style="list-style-type: none"> Evaluate (and communicate) existing model base (E) 		Government, Industry (NETL) with Industry and Academia	<ul style="list-style-type: none"> Consider concurrent engineering Support Vision 21 virtual plant demonstration prototyping
	<ul style="list-style-type: none"> Different groups to do different models electrochemical, kinetic, etc. (R) Develop design/applications models that address SECA vision (D) Incorporate into overall system model (E) 	<ul style="list-style-type: none"> Refine models as necessary (input from benchmarks) (D) <ul style="list-style-type: none"> Accommodate technical breakthroughs Modeling to accommodate markets (implement models P/E we have developed) (D/E) Reduce the turn-around time to speed the design cycle (D) 	Government initiates, develops consortium of government, industry, academia; academia or national lab appointed to coordinate	
BENCHMARK DEVELOPMENT <ul style="list-style-type: none"> >1 Group development and characterize same cell design >1 Group test cell and provide detailed data >4 Groups model 	<ul style="list-style-type: none"> Develop and characterize benchmark cells (D/E) 		Government with academia	none
	<ul style="list-style-type: none"> Test and provide detailed data (D/E) 		Government with academia	
	<ul style="list-style-type: none"> Model (D/E) 		Government with academia and industry	
MODEL SOFC OPERATION (START UP, PART LOAD, SHUT DOWN)	<ul style="list-style-type: none"> Establish off-design conditions and requirements (E) 		Industry with government	none
	<ul style="list-style-type: none"> Development coupled transient models (D/E) 		Government with academia	
	<ul style="list-style-type: none"> Validate model (D/E) 		Government with industry	
		<ul style="list-style-type: none"> Integration with design cycle (E) 	Industry	
		<ul style="list-style-type: none"> Accommodate technology breakthroughs (D/E) 	Government with Academia and industry	

Key: E = Engineering
D = Development
R = Research

Modeling and Simulation: Report-Out

ISSUES	R&D OPPORTUNITIES	ACTIONS
<ul style="list-style-type: none"> • System modeling <ul style="list-style-type: none"> - Total life cycle cost performance analysis optimization • Stack Models <ul style="list-style-type: none"> - lack of suitable multi-physics engineering models (thermal, electrochemical, transport coupling) • Cross-cutting Issues <ul style="list-style-type: none"> - Validation/benchmark data for models 	<ul style="list-style-type: none"> • Stack computational <ul style="list-style-type: none"> Coupled multi-dimensional Multi-physics engineering model (with benchmark problem set) • Cell Computational <ul style="list-style-type: none"> Fundamental models (multi-dimensional) with emphasis on: <ul style="list-style-type: none"> ! Electrochemical ! Kinetic ! Transport aspects • Benchmarks <ul style="list-style-type: none"> - Characterize cell design - Obtain detail test data - Develop model 	<ul style="list-style-type: none"> • Models for Cell /stack <ul style="list-style-type: none"> ! 0-5 Years, Evaluate existing models, G/I ! 0-5 Develop electrochemical, kinetic, models G/I ! 0-5, Application models for SECA vision G/I ! 0-5, Incorporate into system Model G/I ! 5-10 Refine models (for tech. Breakthroughs) G/I ! 5-10 Market-specific models G/I ! 5-10 Reduce turnaround time to speed design cycle G/I • Benchmark <ul style="list-style-type: none"> ! 0-5 Develop/characterize benchmark cells G ! 0-5 Test and provide detailed data G/A ! 0-5 Model development G/A/I • SOFC Operation Model <ul style="list-style-type: none"> ! 0-5 Establish off-design conditions/requirements I ! 0-5 Develop transient model G ! 0-5 Validate model G/I ! 5-10 Integrate with design cycle I ! 5-10 Accommodate technical breakthrough G

Key: I = Industry
 G = Government
 A = Academia

VI. POWER ELECTRONICS

GROUP SUMMARY

Issues

The following issues received the most votes:

- Complex system interface
- Modular family architecture
- Poor load following
- Use of SiC – silicon carbide
- Cooling thermal management
- Lifetime
- Cost discrepancy

Opportunities

The R&D opportunities were categorized into four header topics. The following are the header topics and the corresponding R&D opportunities that received a multiple number of votes:

Thermal Management

- Higher temperature components, e.g., capacitors

Interface

- Integrated devices
- Systems dynamic modeling

Cost

- DFMA –design for manufacture and assembly

Reliability

- Improve component materials

Actions

By combining the component opportunities, actions were developed for the top two opportunities.

Integrated Devices Interface:

- Align with manufacturer
- Develop open architecture for common module hardware and software toolkits

-
- Identify common denominators from developers across applications
 - Assess packaging interconnections
 - Develop codes and standards across industries
 - Develop communication protocols
 - Develop predictive controls

Components Reliability and Thermal Management:

- All components need to be better, faster, smaller, and cheaper
- Re-engineer capacitor
- Improve higher temperature capabilities for connections, solder, circuit boards, and substrate
- Improve switching characteristics with lower losses and higher temperature
- Improve heat sink integrated thermal management

POWER ELECTRONICS

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* = Presenter for report-out

Power Electronics: What Are the Scientific and Technical Issues to Achieve SECA Vision by 2010?

(K = Vote for Priority Topic)

INTERFACE	TOPOLOGY	RELIABILITY	COST
<ul style="list-style-type: none"> • Domain vs. stationary • Synchronize to grid kk • Complex system interface kkkkkkkk • Dynamic range • System inverter ganging • Output power quality • BOP – Balance of Plant • Modular family architecture kkkkkkk • Integrated controls • DC chopper • Programability on fly • Remote dispatch • Black start • Lousy load following kkkkkk 	<ul style="list-style-type: none"> • Switches topology k • Passive components k • SiC – Silicon Carbide kkk 	<ul style="list-style-type: none"> • Cooling thermal management kkkkkk • Graceful degradation • Noise control • Lifetime kkkkkk • Telemetry remote diagnostics 	<ul style="list-style-type: none"> • Size, volume, and weight kk • Economies of scale • Cost discrepancy kkk

Power Electronics: What Are the R&D Opportunities to Overcome Issues to SECA?

(K = Vote for Priority Topic)

THERMAL MANAGEMENT	INTERFACE	COST	RELIABILITY
<ul style="list-style-type: none"> Higher temperature components, e.g., capacitors K K K K K Direct cooling of silicon or SiC K Cheap diamond film Integrated electronic within cell K 	<ul style="list-style-type: none"> Definition of system requirements K K Load prediction Establish standards Challenge 5 kW choice Plug and Play K K Low cost storage high density caps Systems dynamics modeling K K K Functional tradeoff studies Integrated devices K K K K K K K Ganging inverters 	<ul style="list-style-type: none"> Cost tradeoffs studies K Soft switching topology Integrated devices K K Manufacturing process development DFMA K K K K Grid interconnect standards Packaging of PE module 	<ul style="list-style-type: none"> Improve component materials K K K K K K K Prognostics Topology choice, e.g., redundancy, multi-level K Robust design K Soft failure

Power Electronics: What Actions to Take Advantage of R&D Opportunities?

R&D OPPORTUNITY	ACTIONS 0-5 YEARS	TYPE OF ACTION	ACTIONS 5-10 YEARS	TYPE OF ACTION	LEAD ROLES
<ul style="list-style-type: none"> Integrated Devices "Interface" <ul style="list-style-type: none"> ! Board or chip module ! Fuel cell electronics with power electronics ! Transformerless design ! PE-DC Bus in box; PE-AC-Grid outside 	<ul style="list-style-type: none"> Align with manufacturer 	E			<ul style="list-style-type: none"> Industry
	<ul style="list-style-type: none"> Develop open architecture for common module hardware and software toolkits 	E,D			<ul style="list-style-type: none"> Industry, University, Government
	<ul style="list-style-type: none"> Identify common denominators from developers across applications 	E			<ul style="list-style-type: none"> University, Government
	<ul style="list-style-type: none"> Packaging interconnections 	E,D,R			<ul style="list-style-type: none"> Industry, University, Government
	<ul style="list-style-type: none"> Develop codes and standards across industries 	E			<ul style="list-style-type: none"> Government, University, Industry
	<ul style="list-style-type: none"> Communication protocols 	E,D			<ul style="list-style-type: none"> Government, University, Industry
	<ul style="list-style-type: none"> Predictive controls 	E,D,R			<ul style="list-style-type: none"> Government, University, Industry
<ul style="list-style-type: none"> Improve Component Materials "Reliability" and Higher Temperature Components, "Thermal Manage" <ul style="list-style-type: none"> ! Capacitors-inductors ! Connections ! Switch ! Solder ! Circuit boards ! Substrates ! Heat sinks 	<ul style="list-style-type: none"> Better, faster, smaller, cheaper 	D,R	<ul style="list-style-type: none"> Better, faster, smaller, cheaper 	E,D	<ul style="list-style-type: none"> Government, University, Industry
	<ul style="list-style-type: none"> Re-engineer capacitor 	R	<ul style="list-style-type: none"> Re-engineer capacitor 		<ul style="list-style-type: none"> Government, University, Industry
	<ul style="list-style-type: none"> Higher temperature capabilities <ul style="list-style-type: none"> ! Connections ! Solder ! Circuit Boards ! Substrate 	D,R	<ul style="list-style-type: none"> Higher temperature capabilities 	E,D	<ul style="list-style-type: none"> Government, University, Industry
	<ul style="list-style-type: none"> Switch <ul style="list-style-type: none"> ! Improved switching characteristics ! Lower losses ! Higher temperature 	D,R	<ul style="list-style-type: none"> Switch 	E,D	<ul style="list-style-type: none"> Government, University, Industry
	<ul style="list-style-type: none"> Heat sink-integrated thermal management 	D,R	<ul style="list-style-type: none"> Heat sink 	E,D	<ul style="list-style-type: none"> Government, University, Industry

Key: E = Engineering
 D = Development
 R = Research

Power Electronics: Report-Out

POWER ELECTRONICS	ISSUES	R&D OPPORTUNITIES	ACTIONS
<ul style="list-style-type: none"> • Is power electronics in the fuel cell “box” or not? • Ganged 5 kW modules are not practical for power electronics? • Status <ul style="list-style-type: none"> ! \$7/kW mobile in 3 years ! 90+% efficiency ! Air-cooled industrial drives 	<ul style="list-style-type: none"> • Complex system interface • Modular family architecture • Lousy load following • Thermal management • Lifetime 	<ul style="list-style-type: none"> • Integrated devices for interface • Reliability – improve component materials • Thermal Management – higher temperature components 	<ul style="list-style-type: none"> • Integrated devices <ul style="list-style-type: none"> ! Align with manufacturers ! Develop open architecture hardware and software ! Identify common denominators from developers ! Develop codes and standards ! Communication protocols • Component materials: capacitors, inductors, connections, switches, solder, circuit boards, substrates, heat sinks <ul style="list-style-type: none"> ! Better ! Faster ! Smaller ! Cheaper

VII. THERMAL SYSTEMS

GROUP SUMMARY

Issues

The following issues received the largest number of votes:

- Thermal enclosure
- Water recovery system
- Air pre-heater cost/performance trade-off
- Excessive heat losses in small high temperature systems
- Afterburner pre-heater
- Waste heat utilization (power generation/co-generation)
- Transient stresses during normal and abnormal events (loss of cooling air)
- Start-up overall speed

Opportunities

The R&D opportunities were categorized into five header topics. The following are the header topics and the corresponding R&D opportunities that received a multiple number of votes:

Water Management Strategy

- Designs using recycled steam

Air Preheater

- Materials and fabrication
- Integrated catalytic combustion
- Configuration – optimize design

Overall Startup Speed

- Reduce thermal capacitance
- Optimize idle mode strategies

Transient Stresses During Normal and Abnormal Events

- Dynamic modeling (transient)

Thermal Enclosure: Material, Design, & Cost

- Better insulating materials
- Optimize compartment design

Actions

Due to time constraints, only two of the highest priority opportunities could be analyzed.

Water Management - Designs Using Recycled Steam:

- System study of onsite/onboard water vs. recycle steam
- Develop designs for water recovery
- Prototype water recovery
- Research ways to recover water without phase change
- Develop design without phase change
- Prototype without phase change

Thermal Enclosure – Better Insulating Materials:

- Optimize design of the compartment
- Study family of applicable materials and select material
- Prototype

THERMAL SYSTEMS

PARTICIPANTS

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Larry Van Bibber*	SAIC
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* = Presenter for report-out

Thermal Systems: What Are the Issues (Science and Technology) to Achieving the Vision?

(K = Vote for Priority Topic)

OTHER	COMPONENTS	INTEGRATION	OPERATING STRATEGIES
<ul style="list-style-type: none"> Sulfur in fuel creates many of the thermal system issues 	<ul style="list-style-type: none"> Materials No high temperature recycle blower available to recycle anode exhaust back to inlet to provide water Thermal enclosure <ul style="list-style-type: none"> ! Materials ! Design ! Cost kkkkkkkk Catalyst and housing material selection driven by temperature Air preheater cost/ performance trade off kkk Air preheater: need high active heat exchange surface area per unit active volume/weight kk Water Recovery System kkkkk (Seals) Maintaining system integrity due to temperature gradients in space and time kk Nox (Emissions) governed by temperature 	<ul style="list-style-type: none"> Excessive heat losses in small high temperature systems kkkk Using afterburner as startup k Waste heat utilization (power generation/co-generation) kkk Reformer/Stack k Afterburner/Preheater kkkk Air cooled fuel cell stack is too difficult to manage Temperature gradients with air flow uniformity, maintenance (Seals) Maintaining system integrity due to temperature gradients in space and time kk NOx (Emissions) governed by temperature 	<ul style="list-style-type: none"> Designing for extremes k Transient stresses during normal and abnormal events (loss of cooling air) kkkkk Thermal/overall operator training, diagnostics Temperature/flow control system kk Startup <ul style="list-style-type: none"> ! Overall speed kkkkk ! Thermal Human Safety ! Noise ! Emissions ! Heat Air cooled fuel cell stack is too difficult to manage Temperature gradients with air flow uniformity, maintenance

Thermal Systems: What Are the R&D Opportunities to Overcome the Issues?

(K = Vote for Priority Topic)

WATER MANAGEMENT STRATEGY	AIR PREHEATER	OVERALL STARTUP SPEED	TRANSIENT STRESSES DURING NORMAL AND ABNORMAL EVENTS	THERMAL ENCLOSURE: MATERIALS, DESIGN, & COST
<ul style="list-style-type: none"> Optimize design Designs using recycled steam K K K K K K K Misc. – Water for fuel processor 	<ul style="list-style-type: none"> Configuration – optimize design K K K Materials and fabrication K K K K Integrated catalytic combustion K K K K 	<ul style="list-style-type: none"> Reduce thermal capacitance K K K K Optimize idle mode strategies K K K Develop robust hardware design K K 	<ul style="list-style-type: none"> Ceramics – improve, toughened K K Improve hardware design K Dynamic modeling (transient) K K K K Controls design K 	<ul style="list-style-type: none"> Better insulating materials K K K K K Cheaper materials K K Optimize compartment design K K K K

Thermal Systems: What Are the Actions to Take Advantage of the R&D Opportunities

OPPORTUNITY – WATER MANAGEMENT – DESIGNS USING RECYCLED STEAM	ACTION	ACTION TYPE	TIMEFRAME	LEADER	OTHER FACTORS
	System study onsite/onboard water vs. recycle steam	E	6 mo.	DOE/DoD	
	Develop designs for water recovery	E	18 - 24 mos.	Core Tech	
	Prototype (water recovery)	E	1 – 3 yr.. (parallel to research)	Industry	
	Research ways to recover water without phase change	R	1 – 3 yr..	Core Tech	
	Develop design (without phase change)	E	1 - 3 yr..	Core Tech	
	Prototype (without phase change)	E	1 – 3 yr..	Industry	
OPPORTUNITY – THERMAL ENCLOSURE – BETTER INSULATING MATERIALS	ACTION	ACTION TYPE	TIMEFRAME	LEADER	OTHER FACTORS
	Optimize Design	E	1 – 2 yr.	Industry	Note: What must be in the box? 1 – Main box design 2 – Feed platelets
	Study family of applicable materials Select Material	D	6 mos. – 1 yr.	Core Tech	
	Prototype	E	1 – 2 yr.	Industry	

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Thermal Systems – Report Out

(K = Vote for Priority Topic)

Thermal Systems	Issues	Opportunities
<ul style="list-style-type: none"> Thermal Systems What are they? Everything Else <ul style="list-style-type: none"> Air Preheater After burner Thermal enclosure H₂O management Et al. Could be the Achilles Heel 	<ul style="list-style-type: none"> Categories <ul style="list-style-type: none"> Components Operating Strategies Integration Top Vote Getters <ul style="list-style-type: none"> Thermal enclosure K K K K K K K K Air preheater K K K K K K Transients during normal & abnormal events K K K K K K Overall startup rate K K K K K K H₂O recovery system K K K K K K 	<ul style="list-style-type: none"> Categories <ul style="list-style-type: none"> Air preheater Overall startup speed Transients Stresses Thermal enclosure H₂O Management Strategies Top Vote Getters <ul style="list-style-type: none"> Design of H₂O management system using recycled steam K K K K K K K K Better insulating materials for thermal enclosure K K K K K K Optimize compartment design K K K K K K Air preheater materials and fabrication K K K K K K Integrated catalytic combustor with air preheater K K K K K K Reduced thermal capacitance K K K K K K Dynamic modeling K K K K K K

Opportunity	Actions	Timeframe	Lead	Other
<ul style="list-style-type: none"> Water Management Designs Using Recycled Steam 	<ul style="list-style-type: none"> System Study: (E) On board Water vs. Recycle Steam 	6 months	DOE/DoD	
	<ul style="list-style-type: none"> Develop Designs for Water Recovery (E) 	18 - 24 months	Core Tech	
	<ul style="list-style-type: none"> Prototype (E) (water recovery) 	1 – 3 years	Industry	
	<ul style="list-style-type: none"> Research Ways to Recovery Water Without Phase Change (R) 	1 – 3 years (parallel to above)	Core Tech	
	<ul style="list-style-type: none"> Develop Design (E) (without phase change) 	1 – 3 years	Industry	
	<ul style="list-style-type: none"> Prototype (E) (without phase change) 	1 – 3 years		
<ul style="list-style-type: none"> Thermal Enclosure – Better Insulating Materials 	<ul style="list-style-type: none"> Optimize Design 	1 – 2 years	Industry	<ul style="list-style-type: none"> What must be in the box? <ul style="list-style-type: none"> Main box Feed platelets
	<ul style="list-style-type: none"> Study Family of Applicable Materials Select Material 	6 mos. – 1 year	Core Tech	
	<ul style="list-style-type: none"> Prototype 	1 – 2 years	Industry	

Key: E = Engineering
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